UNIVERSIDAD CARLOS III DE MADRID

COMPUTATION OF INERTIAL PARTICLE TRAJECTORIES IN STEADY STREAMING FLOWS

DEPARTMENT OF THERMAL AND FLUIDS ENGINEERING

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Aerospace engineering

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Abstract

The current project consists on the calculation of the inertial particle trajectories in steady streaming flows, implementing the trajectory Maxey-Riley equation through a numerical method in Matlab software. The steady streaming flow is obtained by assuming small oscillation amplitude of an oscillating flow around a set of cylinders. The steady streaming velocity field is calculated through the FreeFem++, a finite element method software. A study of the Maxey-Riley equation is done, in which the different terms of the equation are explained. Using the Euler's Method, the numerical trajectory is developed, choosing one cylinder configuration in order to do a study about the effects of varying parameters such as streaming Reynolds number, fluid-to-particle density ratio, the dimensionless oscillation amplitude and the particle-to-cylinder radius ratio in order to do a summary of the conditions in which the particles are trapped in the streaming flow.

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CHAPTER 1

Introduction

1.1. Background

In recent years, techniques for separating, transporting and trapping small-sized particles in an aqueous environment have emerged motivated by biotechnological needs, such as cell processing and microfluidic devices.

Microfluidics is a field where engineering, chemistry, physics, nanotechnology, biotechnology, and biochemistry are combined with practical issues to design systems in which the fluids are processed. It is used in the development of inkjet printheads, lab-on-a-chip technology, or DNA chips, among others. It consists in the behaviour and precise manipulation and control of fluids with a small (sub-millimeter) scale. Normally, the characteristics of “micro” are small size and volume and low energy consumption[1].

In many biotechnological applications, an important step is the microparticles maintenance at a fixed position in space for their later investigation. Normally, small particles or cells are manipulated with the *patch-clamp technique*, which is based on a micro-pipetting technique that allows trapping a single particle. The disadvantages of this method are that it is laborious, the process is slow and it cannot be automated, so it is inadequate for a lot of biotechnological operations. One application that has emerged in the last years is the μTAS (micro Total

Analysis Systems) or lab-on-a-chip devices, which are microfluidic devices whose role is to automate some biological testing.

The trapping method should have good spatial resolution (the places where particles are maintained must be well located) and the complexity and cost of the whole system should be as small as possible. Additionally, trapping methods must not affect the state of the particle because some particles such as living cells are very delicate, and therefore the contact with solid object must be avoided. The methods can be classified as direct contact methods and non-contacting methods[2].

The direct contact method with the particle might produce an undesired mechanical stress that may cause a loss of the functionality of the object.

The non-contacting methods do not have that problem and they can be categorized according to the physical mechanism that is used to attract and maintain the particles to a certain position. The main methods are:

- **Optical tweezers**: laser-based system used to guide single particles to a certain positions. This method is very accurate but the cost is high and the laser beam could have a negative effect on some particles.
- **Dielectrophoretic trapping**: it uses the polarizability of the particles to form a trapping force due to the action of non-uniform electric field. The disadvantages are that is a too expensive method and the effect on living particles can be a problem.
- **Magnetic trapping**: this method only works with particles with magnetic properties.
- **Acoustic trapping**: it takes advantage of the radiation forces on a particle located in an ultrasonic wave, moving the particle to the nodes of the waves. This method is cheaper than the others.

- **Hydrodynamic trapping**: it uses an adapted flow field in order to bring the particle to a certain spatial positions, where it eventually will stay trapped. Normally, this is obtained through a flow configuration called microeddy, in which the particle is guided in a spiralling trajectory to the centre of the eddy. One way to create microeddies is taking advantage of the steady streaming that is produced by the oscillation flow around solid objects. It is probed that the trapping force is greater when the Reynolds number is higher. The present project is based on this trapping method to obtain the trajectories.

1.2. Goals of the project

The main goal of this project is to calculate the inertial particle trajectories in steady streaming flows, through a numerical method implemented in Matlab software. In order to reach this objective, it is necessary to achieve some secondary goals. They have been specified as:

- Understand the steady streaming flow and its behaviour.
- Interpret the FreeFem++ results of the steady streaming around a set of cylinders.
- Develop a numerical method in Matlab to calculate the trajectories based on the Maxey-Riley equation.
- Analyse the effects of the parameters such as Reynolds number, fluid-to-particle density ratio and the particle-to-cylinder radius, among others.

1.3. Project planning and budget

Once the objectives of the project are shown, a project planning is developed taking into account the phases in which this project has been carried out. Firstly, it is necessary to search and understand about the background of the trapping methods and previous experiments. Then, in order to calculate the trajectory of a small spherical particle, the Maxey-Riley equation must be studied and understood. To calculate the potential flow of the different cylinder configurations and the steady streaming flow generated for the oscillated flow around the cylinders, FreeFem++ is used, so it is necessary to understand how to work with the data obtained in this FEM software. The next step is to develop the numerical code in Matlab using Euler's Method. Once the results are shown, interpreting them to obtain the conclusions is the following phase. Besides, periodical meeting with the tutor to be assisted are included. Finally, writing the report is the last step.

The global invested time has been around 3 months. Now, the distribution of work hours needed to develop each phase is as follows:

Project phases	Work hours
Searching and understanding the researched literature	30
Theoretical study of the Maxey-Riley equation	40
Understanding FreeFem++ output results	20
Numerical method implemented in Matlab	60
Getting results	20
Interpreting results and getting conclusions	60
Periodical meeting	30
Writing the report	80
Revision and correction of the final report	10
Total time	**Total time**

Table 1. Project phases

Once the work planning has been described, a virtual budget is proposed (see Table 2), taking into account the different expenses needed to carry out the project, the normal wage of an engineering and the licence of the Matlab software. Additional expenses contain the technological equipment and other issues necessary to perform the project such as computer and travel expenses.

Project phases	Time	Cost
Engineering work (30€/h)	350 hours	10,500€
Annual licence for Matlab (2000€/$year$)	3 months (0.25 years)	500€
Additional expenses	-	1,000€
Total		**12,000€**

Table 2. Project budget

1.4. Contents of the project

This project is organised in four chapters, taking into account the different steps of the research, as follows:

In the first chapter, it is provided an introduction of the global issues of the techniques for separating, transporting and trapping small-sized particles. The main techniques are presented (contact and non-contact), where advantages and disadvantages are described. There is a second statement in which the goals of the project are listed. The third part of the introduction deals with the project planning, where all the steps in which the project has been divided and the time required to perform each step are defined. In addition, a virtual budget of the project is explained. Finally, an outline is provided to present the contents of each chapter.

The second chapter is related to the methodology. To begin with, the theoretical background is described, explaining the concepts about steady streaming flow, the Maxey-Riley equation development (equation of motion for a small rigid sphere in a non-uniform flow) and each of its terms (added mass, viscous Stokes drag…). In addition, the numerical method to calculate inertial particle trajectories is introduced. Firstly, it is mentioned the use of FreeFem++ software (using finite elements) to solve the oscillating flow. Secondly Euler's Method is implemented in Matlab software (high-level language and interactive environment for numerical computation) to be concerned with the numerical solution of the Maxey-Riley equation.

The third chapter presents the results of the trajectories for one chosen configuration (changing the position of the cylinders) and different parameters such as streaming Reynolds number, fluid-to-particle density ratio and the particle-to-cylinder radius ratio, among others.

In the fourth chapter the main conclusions are exposed, taking into account the results obtained in the previous section and the comparison with other numerical calculation of other authors, in order to optimize the best configuration to trap microparticles. Future works are included in this section.

Finally the references are cited, containing the principal papers and sources of information used in the project.

CHAPTER 2

Methodology

2.1. Theory

In this part, a theoretical study of the problem is analysed in order to solve it in a numerical way in the next section. Firstly, the concept of the steady streaming flow and the solution of an oscillatory flow around cylinders are briefly developed[3]. Secondly, there are introduced the Maxey-Riley equation, the previous studies where it comes from, the definition of each term of the equation and its limitations.

2.1.1. Steady streaming around a set of cylinder because of an oscillatory flow

Considering a set of four equal (a) radius cylinders placed as sketched in *Figure 1*, and separated between them a fixed distance g. There is an oscillatory flow around the cylinders, whose velocity magnitude is $Ucos(wt)$ and it is perpendicular to the line that connects the centres of the horizontal cylinders.

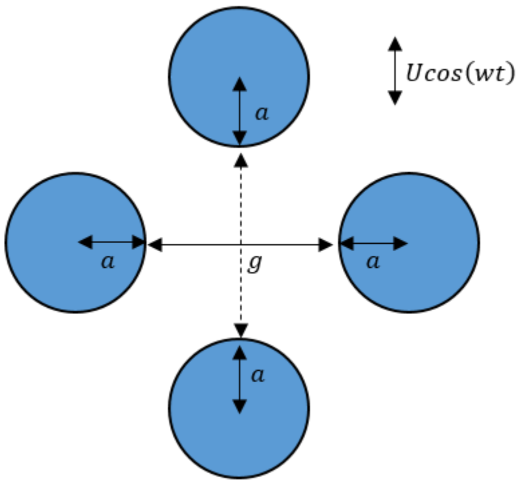

Figure 1. Cylinder configuration

Other important parameters are: $d = U/w$, which measures the amplitude of displacement of the particles in the oscillating flow; and $\delta = \sqrt{\nu/w}$, which measures the thickness of the Stokes layer at the cylinder's surface. The Stokes boundary layer refers to the boundary layer close to a solid non-oscillatory wall flow of a viscous fluid[4]. A streaming flow is a weak but large steady response of a fluid to a non-linear interaction in a dominant oscillatory flow. Those non-linear interactions, in this case the Reynolds stresses in the cylinder's surface, produce a time-independent streaming motion that lasts beyond the Stokes layer and cause a streaming motion with a velocity of lower magnitude than the oscillating magnitude U.

Using *a*, *U*, and w^{-1} as characteristics length, velocity and time scale, respectively, the three dimensionless parameters that control the flow are as follow:

$$\varepsilon = \frac{U}{wa} = \frac{d}{a} \tag{2.1}$$

$$Re_s = \frac{U^2}{w\nu} = \frac{\varepsilon U a}{\nu} \tag{2.2}$$

$$g_a = \frac{g}{a} \tag{2.3}$$

Where ε is the dimensionless oscillation amplitude, which in this project is assumed to be smaller than unit ($\varepsilon \ll 1$).

The streaming Reynolds number Re_s, is based on the velocity of the steady streaming. g_a is the ratio between the distance among cylinders and the cylinder's radius. In the regime $Re_s \gg 1$, is where the strongest microeddies are generated, so the trapping forces are higher. As $Re_s = \varepsilon Re$, this case is categorized in the 2 boundary layer (Stuart, Riley) regime, as sketched in *Figure 2*. It is in this regime where the project is focused, taking into account that this regime has not been studied before due to the difficulties of controlling this flow. Because of the fact that this is a new method for trapping small particles, there is no any regulation (rules, techniques or constraints) applicable to this method.

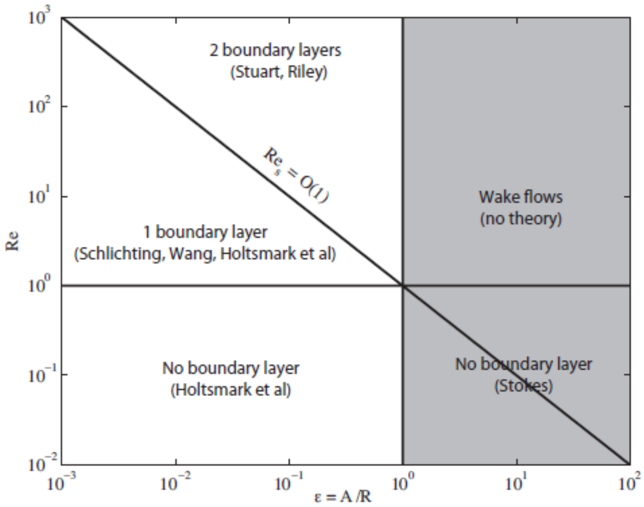

Figure 2. Streaming regimes (adapted from Wang [5])

The kinematic viscosity ν is the ratio between the dynamic viscosity μ and the density of the fluid ρ. It is an important concept when analysing the Reynolds number Re (Dimensionless quantity that is known as the ratio between momentum forces and viscous forces, so it is quantified the relative importance of those forces for a given flow conditions).

$$\nu = \frac{\mu}{\rho} \tag{2.4}$$

$$Re = \frac{\rho u L}{\mu} = \frac{uL}{\nu} \tag{2.5}$$

Where u and L are the characteristic velocity and length, respectively.

When the reference frame is set between the cylinders, the flow is symmetric about both planes x=0 and y=0. To solve the problem, as the normal solution takes much time to calculate it, an approximate method is provided. Taking the limit of $\varepsilon \ll 1$, in which the Stokes layer thickness becomes very small ($\delta/a = \varepsilon/\sqrt{Re_s}$), the stream function can be expanded as:

$$\psi(x,\tau) = \psi_0(x,\tau) + \varepsilon\big(\psi_1(x,t) + \psi_1(x)\big) + H.O.T. \tag{2.6}$$

Where a steady streaming appears (τ is the dimensionless time) .The higher other terms (H.O.T.) are neglected. At leading order, the flow is given by:

$$\psi_0(x,\tau) = \tilde{\psi}_0(x) \cdot cos\tau \tag{2.7}$$

Where $\tilde{\psi}_0$ correspond to the potential flow due to the cylinder configuration, this is because of the thin Stokes layer in which the vorticity oscillations are confined, so outside the layer, the vorticity oscillation might be neglected, so considering the flow velocity oscillations irrotational outside this layer is a good approximation[6].

The boundary conditions are imposed on the cylinder surfaces with the latter velocity obtained by Coenen and Riley (2009)[7]. With this method implemented in FreeFem++, it is possible to obtain the dimensionless velocities and streamlines for different cylinder configurations. The dimensionless velocities have the form:

$$u(x,\tau) = \widetilde{u_0}(x,\tau) + \varepsilon u_1(x) = u_0(x)cos\tau + \varepsilon u_1(x) \tag{2.8}$$

Where u_0 is the velocity obtained from the potential $\tilde{\psi}_0(x)$ and u_1 is the streaming velocity.

2.1.2. Inertial Particle Trajectory

In this section, the equation to solve the motion of a small sphere particle in a non-uniform flow, called Maxey-Riley[8] equation, is presented. Firstly, a briefly introduction about the origin of the formula. Then, the different terms of the equation are explained and which of them could be neglected.

In fluid dynamics, normally the Basset–Boussinesq–Oseen equation (BBO equation) is used to describe the motion of a small spherical particle assuming to be at sufficiently small Reynolds number in unsteady flow. For a small sphere of radius b and mass m_p, instantaneously centred at $\boldsymbol{Y}(t)$, and velocity $\boldsymbol{V_i}(t)$, the BBO equation is (versioned by Corrsin and Lumley):

$$m_p \frac{d\boldsymbol{V_i}}{dt} = m_F \left(\frac{D\boldsymbol{u_i}}{Dt} - \nu \nabla^2 \boldsymbol{u_i} \right) \Big]\Big]_{\boldsymbol{Y}(t)} - \frac{1}{2} m_F \frac{d}{dt} \{ \boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t), t] \}$$
$$- 6\pi b\mu \Bigg(\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t), t] \tag{2.9}$$
$$+ b \int_{-\infty}^{t} d\tau \frac{d/d\tau \{ \boldsymbol{V_i}(\tau) - \boldsymbol{u_i}[\boldsymbol{Y}(\tau), \tau] \}}{[\pi \nu (t-\tau)]^{1/2}} \Bigg) + (m_p - m_F) \boldsymbol{g_i}$$

The undisturbed flow field is $\boldsymbol{u_i}(x, t)$, m_F is the mass of the fluid in the same volume than the sphere, and μ and ν are the dynamic and kinematic viscosity, respectively.

In the equation, there are two kind of time derivatives. The first one represents a time derivative following the moving sphere, so it is the fluid velocity time derivative:

$$\frac{d}{dt}\boldsymbol{u_i}[\boldsymbol{Y}(t),t] = \left(\frac{\partial \boldsymbol{u_i}}{\partial t} + \boldsymbol{V_i}\nabla\boldsymbol{u}\right)\Big]\!\Big] \tag{2.10}$$

The second one denotes the time derivative following a fluid element, it is said, is the fluid acceleration in the centre of the spherical particle.

$$\frac{D\boldsymbol{u_i}}{Dt}\Big]\!\Big]_{\boldsymbol{Y}(t)} = \left(\frac{\partial \boldsymbol{u_i}}{\partial t} + \boldsymbol{u_i}\nabla\boldsymbol{u}\right)\Big]\!\Big] \tag{2.11}$$

This equation is not consistent due to the fact that the effects of pressure gradient of the undisturbed flow are not greater than the effects of viscous shear stress, in fact, they can be comparable. Then the first term should be, as Riley recommends:

$$m_F\left(\frac{D\boldsymbol{u_i}}{Dt}\right)\Big]\!\Big]_{\boldsymbol{Y}(t)} \tag{2.12}$$

In addition, the Faxén correction is added to modify the drag force in the sphere because of the small Reynold number of the particle. Finally the Maxey-Riley equation has the form:

$$\begin{aligned} m_p\frac{d\boldsymbol{V_i}}{dt} = {} & m_F\frac{D\boldsymbol{u_i}}{Dt}\Big]\!\Big]_{\boldsymbol{Y}(t)} - \frac{1}{2}m_F\frac{d}{dt}\left\{\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t),t] - \frac{1}{10}b^2\nabla^2\boldsymbol{u_i}]\!]_{\boldsymbol{Y}(t)}\right\} \\ & - 6\pi b\mu\left(\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t),t] - \frac{1}{6}b^2\nabla^2\boldsymbol{u_i}]\!]_{\boldsymbol{Y}(t)}\right) \\ & - 6\pi b^2\mu\int_0^t d\tau\frac{d/d\tau\left\{\boldsymbol{V_i}(\tau) - \boldsymbol{u_i}[\boldsymbol{Y}(\tau),\tau] - \frac{1}{6}b^2\nabla^2\boldsymbol{u_i}]\!]_{\boldsymbol{Y}(\tau)}\right\}}{[\pi\nu(t-\tau)]^{1/2}} \\ & + (m_p - m_F)\boldsymbol{g_i} \end{aligned} \tag{2.13}$$

Other term that can be added is the Saffman lift force (L), that is used by Chong[2], but this term is only important for specific regions, near the solid surfaces, regions which could change the dynamics of the particle trapping. In general, they are not the dominant effect in the equation of motion, so it can be neglected.

Coming back to the equation 2.13, the different terms that compose this formula are:

- **Fluid acceleration force** (F_{fa}): it is the fluid acceleration in the centre of the spherical particle. It represents the effects of pressure gradients of the undisturbed flow:

$$F_{fa} = m_F \frac{D\boldsymbol{u_i}}{Dt} \Big\rrbracket_{\boldsymbol{Y}(t)} \tag{2.14}$$

- **Added mass force** (F_{am}): the added mass[9] or virtual mass is the inertia added to a system because of the fact that a body with a certain acceleration must move a volume of the surrounding fluid as it moves through it. This phenomenon occurs because the object and surrounding fluid cannot be placed in the same physical space simultaneously. For convenience it could be modeled as some volume of fluid moving with the object:

$$F_{am} = -\frac{1}{2} m_F \frac{d}{dt} \left\{ \boldsymbol{V_i}(t) - \boldsymbol{u}_i[\boldsymbol{Y}(t), t] - \frac{1}{10} b^2 \nabla^2 \boldsymbol{u_i} \rrbracket_{\boldsymbol{Y}(t)} \right\} \tag{2.15}$$

  When the derivative of the particle velocity is moved to the left hand side, it is get that the particle is accelerated as if it has an added mass of half the fluid it moves, and there is a force contribution on the right hand side due to acceleration of the fluid.

- **Stokes drag force** (F_{sd}): it is the frictional force (drag force) that occurs on spherical particles with small Reynolds numbers in a viscous fluid[4]. Other assumptions that are made by Stokes' law are: uniform in composition particle, smooth surfaces and particles do not affect each other. It is the dominant term in the Maxey-Riley equation and it has the form:

$$F_{sd} = -6\pi b\mu \left(\boldsymbol{V_i}(t) - \boldsymbol{u}_i[\boldsymbol{Y}(t), t] - \frac{1}{6} b^2 \nabla^2 \boldsymbol{u_i} \rrbracket_{\boldsymbol{Y}(t)} \right) \tag{2.16}$$

- **Basset history force** (F_{bh}): It is also known as memory term, and it describes the cumulative effect of the diffusion of the vorticity from the particle along its total path[2]. The computation is extremely difficult, so it is normally neglected.

$$F_{bh} = -6\pi b^2 \mu \int_0^t d\tau \frac{d/d\tau \left\{ \boldsymbol{V_i}(\tau) - \boldsymbol{u_i}[\boldsymbol{Y}(\tau), \tau] - \frac{1}{6} b^2 \nabla^2 \boldsymbol{u_i} \rrbracket_{Y(\tau)} \right\}}{[\pi \nu (t-\tau)]^{1/2}} \tag{2.17}$$

- **Gravity force** (F_g): for this project, it is neglected.

$$F_g = (m_p - m_F)\boldsymbol{g_i} \tag{2.18}$$

- **Faxén correction:** all the terms that contain the Laplacian ($\nabla^2 \boldsymbol{u_i}$) are affected by the Faxén corrections, which represents the effects of non-uniform fluid velocity to the inertial particle. Those corrections may be neglected in this project because their contribution is important in regions with significant vorticity, which is almost negligible along the path of the inertial particle.

Finally, the resultant Maxey-Riley equation, which is used in the project, with the simplifications is:

$$\begin{aligned} m_p \frac{d\boldsymbol{V_i}}{dt} = m_F \frac{D\boldsymbol{u_i}}{Dt}\bigg\rrbracket_{\boldsymbol{Y}(t)} - \frac{1}{2} m_F \frac{d}{dt}\{\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t), t]\} \\ - 6\pi b \mu (\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t), t]) \end{aligned} \tag{2.19}$$

Now, dividing the equation between the volume of a spherical fluid particle with the same radius b than the inertial particle ($\frac{4}{3}\pi b^3$), it gives the equation:

$$\rho_p \frac{d\boldsymbol{V_i}}{dt} = \rho_F \frac{D\boldsymbol{u_i}}{Dt}\bigg\rrbracket_{\boldsymbol{Y}(t)} - \frac{1}{2}\rho_F \frac{d}{dt}\{\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t), t]\} - \frac{9\mu}{2b^2}(\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t), t]) \tag{2.20}$$

Where ρ_p is the inertial particle density and ρ_F is the fluid density. Finally, dividing the equation between the particle density and taking into account that η

is the fluid-to-particle density ratio, the formula to be implemented in the numerical method is:

$$\frac{d\boldsymbol{V_i}}{dt} = \eta \frac{D\boldsymbol{u_i}}{Dt}\bigg]\!\!\bigg]_{\boldsymbol{Y}(t)} - \frac{1}{2}\eta\frac{d}{dt}\{\boldsymbol{V_i}(t) - \boldsymbol{u}_i[\boldsymbol{Y}(t), t]\} - \frac{9\eta\nu}{2b^2}(\boldsymbol{V_i}(t) - \boldsymbol{u}_i[\boldsymbol{Y}(t), t]) \qquad (2.21)$$

It is important to mention that the flow follows an Eulerian[4] specification, which is a way of seeing the fluid motion based on specific locations in the space in which the fluid moves as time passes.

Finally, one way to determine the inertia of a particle is to calculate the Stokes number, which is a dimensionless parameter proportional to the inertia. It is defined as:

$$St = \frac{2U_0 b^2}{9\eta\nu a} \qquad (2.22)$$

Where U_0 is the characteristic velocity and a is the characteristic length (in this case it is the radius of the cylinder). If it is calculated the dimensionless equation and introducing the Stokes number, it will be:

$$St\frac{d\boldsymbol{V}}{d\tau} = St\eta\frac{D\boldsymbol{U}}{D\tau} - \frac{St\eta}{2}\frac{d}{d\tau}(\boldsymbol{V} - \boldsymbol{U}) - (\boldsymbol{V} - \boldsymbol{U}) \qquad (2.23)$$

When the Stokes number is small, it results in a low difference between the velocity of the particle and the local fluid, so the inertial particle follows almost a fluid particle (particle with no inertia) trajectory.

2.2. Numerical method

After the theoretical part, the numerical method is development. The first section mentions the main software used to solve the project's problem. Then the Euler's method is briefly explained, and finally, the implementation of the Maxey-Riley equation in Matlab is described.

2.2.1. Software

In order to solve a great variety of engineering problems, it is used the Finite Element Method (FEM). It is a numerical procedure for getting approximate solutions with reasonable accuracy of complex problems were analytical solutions are difficult to obtain. FEM models a structure by discretizing it into a smaller unit, finite elements, that are connected between them by points called nodes.

To calculate the potential flow of the different cylinder configurations and the steady streaming flow generated for the oscillated flow, the FreeFem++ software is utilized.

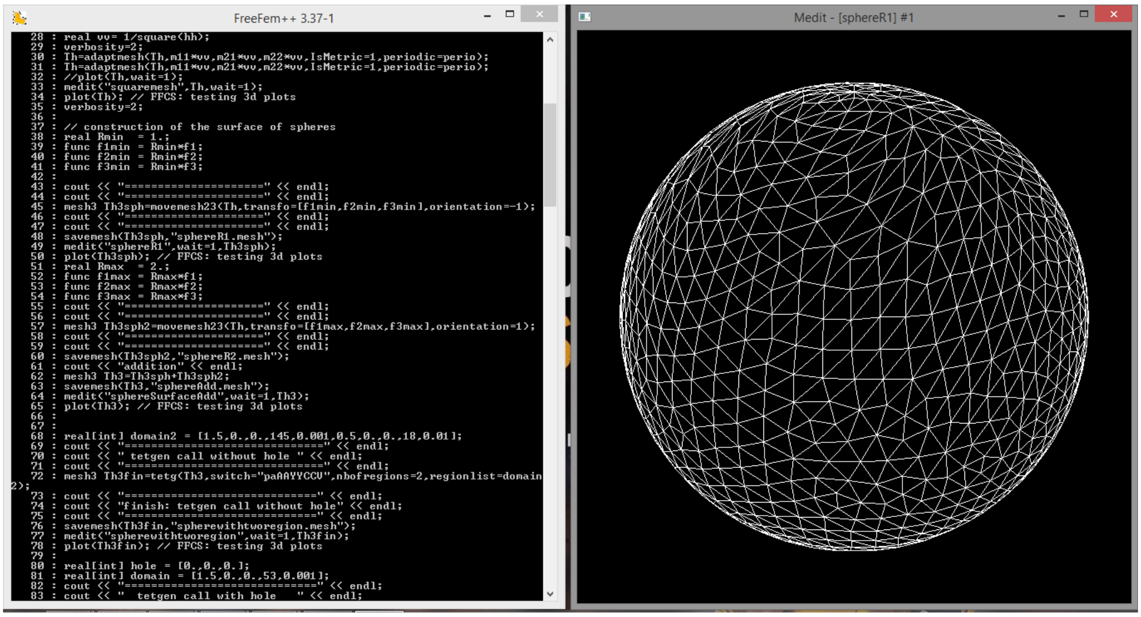

Figure 3. Interface of the FreeFem++

FreeFem++[10] is a programming language and a software focused in solving partial differential equations using the finite element method. It is written in C++ and developed and maintained by Université Pierre et Marie Curie and Laboratoire Jacques-Louis Lions. It runs on GNU/Linux, Solaris, OS X and MS Windows systems. FreeFem++ is free software. The first version was created in 1987 by Olivier Pironneau.

As FreeFem++ software has not an easy interface, and it is difficult to work with it, the solution is to work with an integrated environment which provides more intuitive graphical interface to the users. The used software is the FreeFem++-cs[11], which also gives extra features such as: color-coded editor, integrated graphic area for 2D and 3D, automatic highlighting of compilation error, among others.

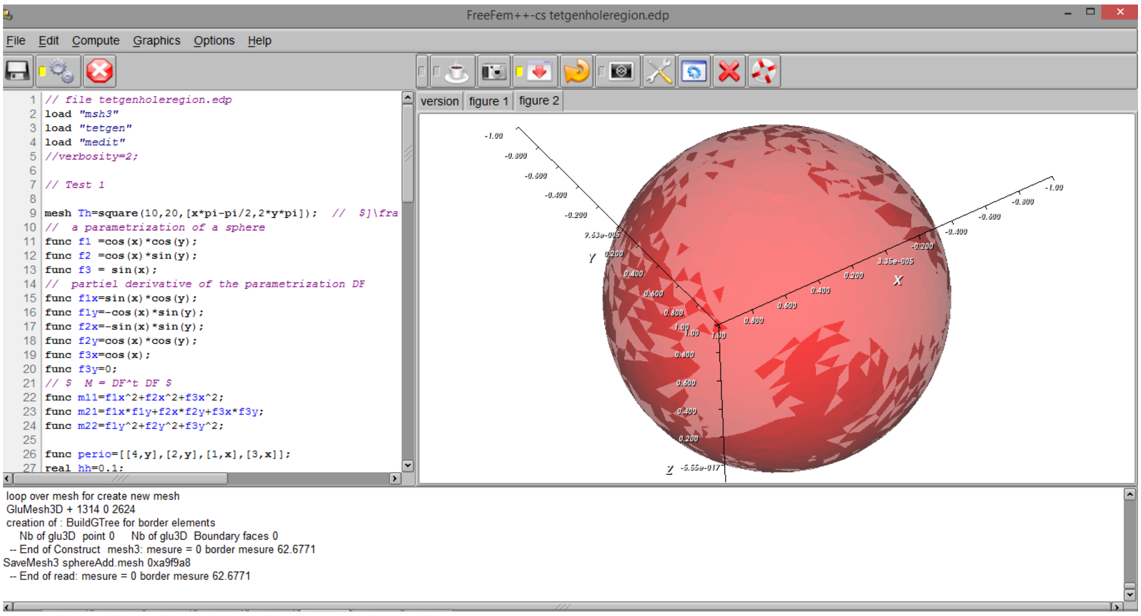

Figure 4. Interface of the FreeFem++-cs

To implement the numerical method, the used tool is Matlab[12] software, which is a high-level language and interactive environment for numerical computation, visualization, and programming. Using MATLAB, it can be analysed data, developed algorithms, and created models and applications. The language, tools, and built-in math functions enable to explore multiple approaches and reach a solution faster than with spreadsheets or traditional programming languages, such as C/C++ or Java®. Matlab can used for a range of applications, including signal processing and communications, image and video processing, control systems, test and measurement, computational finance, and computational biology. More than a million engineers and scientists in industry and academia use MATLAB, the language of technical computing. The most important key features are:

- High-level language for numerical computation, visualization, and application development.
- Interactive environment for iterative exploration, design, and problem solving.
- Mathematical functions for linear algebra, statistics, Fourier analysis, filtering, optimization, numerical integration, and solving ordinary differential equations.
- Built-in graphics for visualizing data and tools for creating custom plots.
- Development tools for improving code quality and maintainability and maximizing performance.
- Tools for building applications with custom graphical interfaces.
- Functions for integrating MATLAB based algorithms with external applications and languages such as C, Java, .NET, and Microsoft Excel.

2.2.2. Euler's Method

To implement the numerical solution in Matlab, Euler's Method[13] is used. This method is a numerical procedure to solve ordinary differential equation (ODEs) with a given initial value. Euler's Method is a basic explicit method (it means that calculate the state of a system at a later time from the state of the system at the current time). In this method, the error per step (local error) is proportional to the square of step size, while the error at a given time (global error) is proportional to the step size.

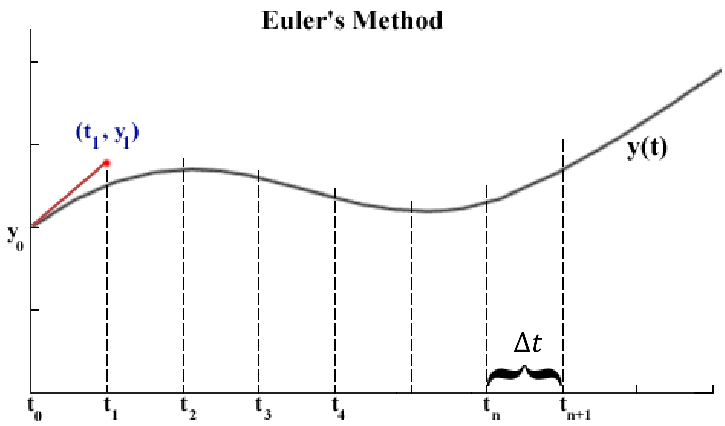

Figure 5. Euler's Method

$$y'(t) = f(t, y(t)) \tag{2.24}$$

$$y(t_0) = y_0 \tag{2.25}$$

Now, it is necessary to choose a value of the size of each step (Δt), such that:

$$t_{n+1} = t_n + \Delta t \tag{2.26}$$

$$y_{n+1} = y_n + \Delta t \cdot f(t_n, y_n) \tag{2.27}$$

The Euler method is more detailed when the step size is lower, but the total number of steps increases, so the step size selection should be studied taking into account the relation between the accuracy and the calculation time.

For the derivative calculation, the possibility is to consider the Taylor expansion of the function.

$$y(t_0 + \Delta t) = y(t_0) + \Delta t \cdot y'(t_0) + \frac{1}{2}\Delta t^2 y''(t_0) + O(\Delta t^3) \tag{2.28}$$

Ignoring the quadratic and higher-order terms, the derivative can be substitute by:

$$y'(t_0) \approx \frac{y(t_0 + \Delta t) - y(t_0)}{\Delta t} \tag{2.29}$$

For this project, this method is used for time derivatives.

2.2.3. Assessment of the trajectory equation

In order to calculate the trajectory, the first step is to choose the parameters Re_s (streaming Reynolds number), ε (dimensionless oscillation amplitude), a (cylinder radius), η (fluid-to-particle density ratio) and b/a (particle-to-cylinder radius ratio). Then the cylinder configuration is set. With those parameters it is possible to obtain the rest of terms using equations 2.1 and 2.2 as follows:

$$U = \frac{Re_s \nu}{\varepsilon a} \tag{2.30}$$

$$w = \frac{U}{\varepsilon a} \tag{2.31}$$

$$T = \frac{2\pi}{w} \tag{2.32}$$

Where U is the characteristic velocity, w is the angular velocity of the oscillations and T is the period of the oscillation. The last two terms are important to select the time step.

As the FreeFem++ results are presented in a dimensionless way, taking the characteristic values of velocity U it is possible to obtain the dimensional solutions. The initial conditions for the velocity of the inertial particle are set as the surrounding fluid in the same position:

$$\boldsymbol{V_i}(t=0) = \boldsymbol{u_i}[\boldsymbol{Y}(t=0), t=0] \tag{2.33}$$

Finally the equations of motion implemented in Matlab are:

$$\boldsymbol{a_i} = \frac{d\boldsymbol{V_i}}{dt} = \frac{\left(\eta \frac{D\boldsymbol{u_i}}{Dt}\Big]\!\Big]_{Y(t)} + \frac{1}{2}\eta \frac{d}{dt}\{\boldsymbol{u_i}[\boldsymbol{Y}(t),t]\} - \frac{9\eta\nu}{2b^2}(\boldsymbol{V_i}(t) - \boldsymbol{u_i}[\boldsymbol{Y}(t),t])\right)}{\left(1+\frac{1}{2}\eta\right)} \tag{2.34}$$

$$\boldsymbol{V_i} = \frac{d\boldsymbol{Y_i}}{dt} \tag{2.35}$$

$$\boldsymbol{V_i}(t_0 + \Delta t) = \boldsymbol{V_i}(t_0) + \Delta t \cdot \boldsymbol{a_i}(t_0) \tag{2.36}$$

$$\boldsymbol{Y}_i(t_0 + \Delta t) = \boldsymbol{Y}_i(t_0) + \Delta t \cdot \boldsymbol{V_i}(t_0) \tag{2.37}$$

Where

$$\nabla \boldsymbol{u} = \begin{pmatrix} \left(\frac{\partial u_1}{\partial x_1}\right) & \left(\frac{\partial u_1}{\partial x_2}\right) \\ \left(\frac{\partial u_2}{\partial x_1}\right) & \left(\frac{\partial u_2}{\partial x_2}\right) \end{pmatrix} \tag{2.38}$$

$$\frac{\partial \boldsymbol{u_i}}{\partial t}(t_0) \approx \frac{\boldsymbol{u_i}(t_0 + \Delta t) - \boldsymbol{u_i}(t_0)}{\Delta t} \tag{2.39}$$

$$\frac{\partial \boldsymbol{u_i}}{\partial x_j}(t_0) \approx \frac{\boldsymbol{u_i}(t_0 + \Delta t) - \boldsymbol{u_i}(t_0)}{\boldsymbol{Y_j}(t_0 + \Delta t) - \boldsymbol{Y_j}(t_0)} \tag{2.40}$$

$$\boldsymbol{u_i}(\boldsymbol{Y}_i(t_0 + \Delta t), t_0 + \Delta t) = u_0(x)\cos(w(t_0 + \Delta t)) + \varepsilon u_1(x) \tag{2.41}$$

CHAPTER 3

Results

3.1. Getting started

Firstly to show better the results in the figures, intead of represent the whole trajectory of an inertial particle including the oscillations due to the flow, the trajectory is sampled once per cycle for clarity reasons, as sketched in *Figure 6*.

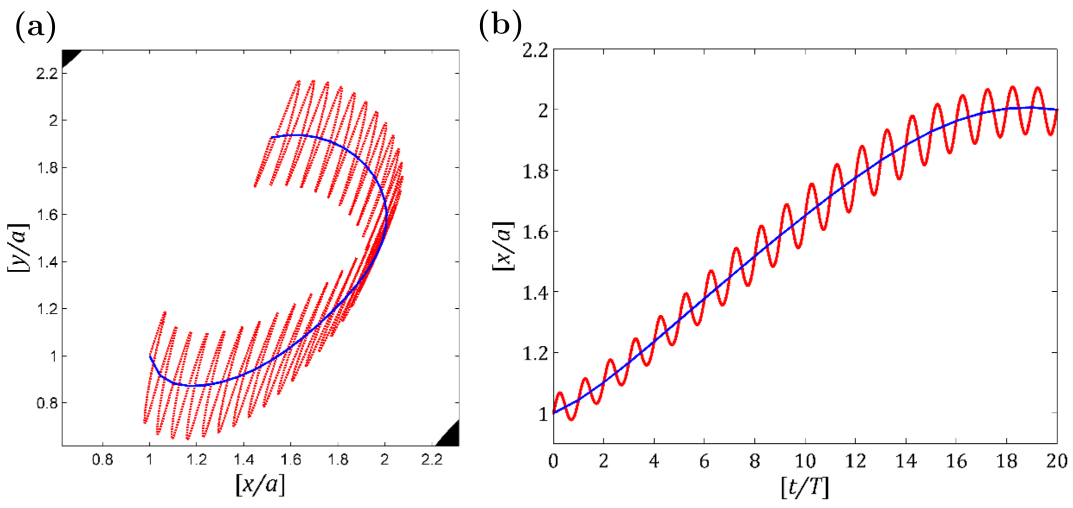

Figure 6. (a) Real inertial particle trajectory (red line), and trajectory when it is sampled once per cycle (blue line). (b) Real X-position variation with time (red line) and X-position variation with time when it is sampled once per cycle (blue line)

3.2. Time step

Other important parameter to keep in mind is the time step used in the calculation of the trajectory that is explained in the section of the Euler's Method. The time step should be as small as possible in order to get accurate results. On the other hand, small time step requires more calculations steps (more time to calculate the trajectory) for the same final time.

To choose the best time step, setting $Re_s = 70$, $\varepsilon = 0.15$, $T \approx 0.2s$ and $a = 1cm$, and using the trajectory of a fluid particle, different trajectories are calculated changing the time step to select the best option. As it can be seen in *Figure 7*, when the value of the step time is lower, the path is increased. There is a remarkable increment until the value of $\Delta t = 0.05T \approx 0.01s$, in which the trajectory is kept almost constant as it is shown in the *Figure 8*. In conclusion, this is a high value of time step that provides a good approximation of the real trajectory, so the total number of time steps is smaller than lower time steps (reducing the total time of calculation).

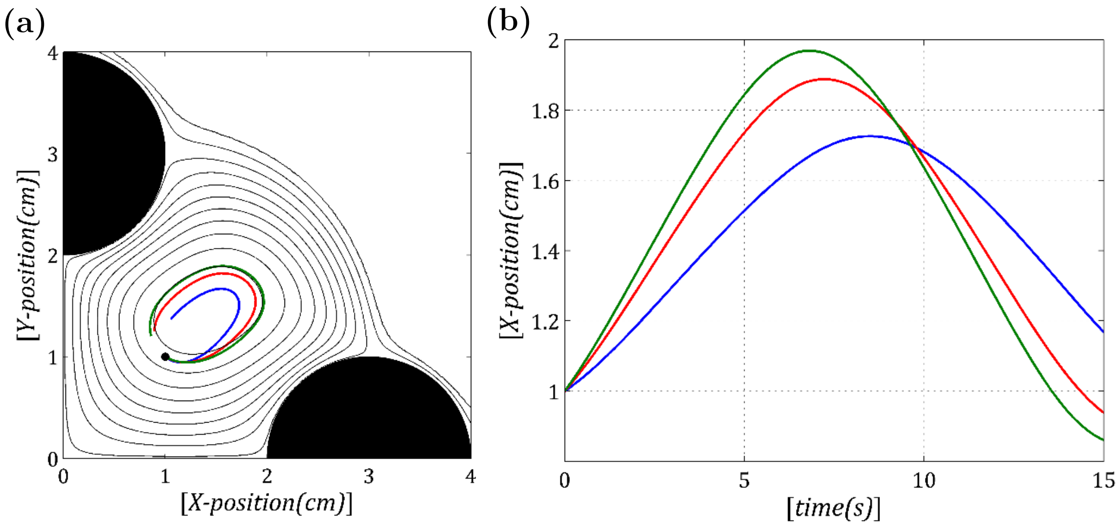

Figure 7. For Res=70, ε=0.15, η=1, T≈0.2s and a=1cm, changing the time step: Δt=0.2T≈0.04s (blue line), Δt=0.1T≈0.02s (red line) and Δt=0.05T≈0.01s (green line). (a) Fluid particle trajectory when it is sampled once per cycle. (b) Fluid particle X-position variation with time when it is sampled once per cycle

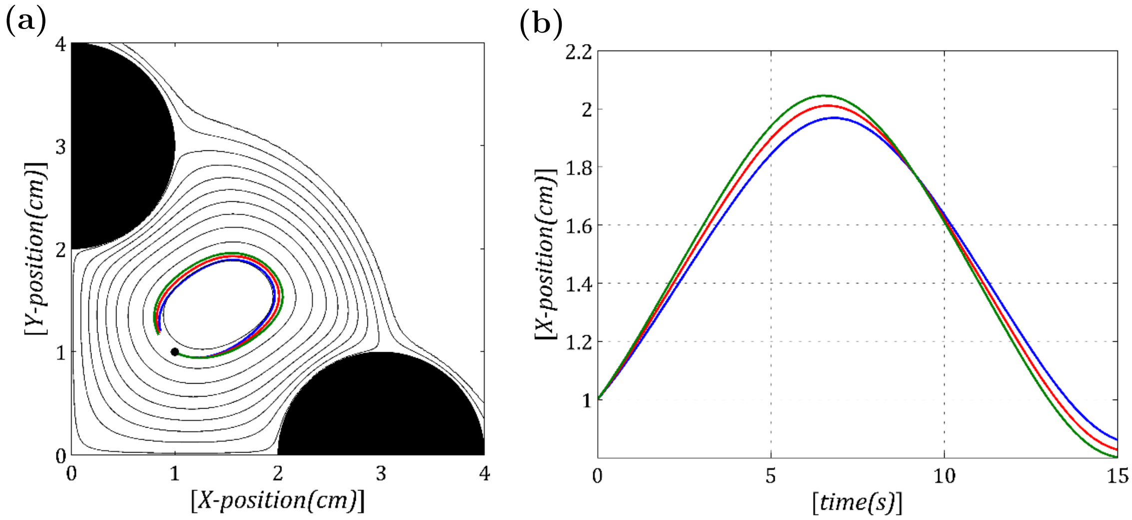

Figure 8. For Res=70, ε=0.15, η=1, T≈0.2s and a=1cm, changing the time step: Δt=0.05T≈0.01s (blue line), Δt=0.025T≈0.005s (red line) and Δt=0.005T≈0.001s (green line). (a) Fluid particle trajectory when it is sampled once per cycle. (b) Fluid particle X-position variation with time when it is sampled once per cycle

3.3. Configurations

Once the time step order has been selected ($\Delta t \approx 0.01s$), taking into account that the time step depends on the period, the cylinder configuration is analysed. Looking the streaming velocity magnitude that are shown in *Figure 9*, in the first and the second configuration, because of the fact that the cylinders are close together there is not an apparent microeddy. Instead of this, smaller microeddies appear, so it will be difficult to place the position of the inertial particle when it is trapped. When the cylinders are far away between them, an evident microeddy is formed.

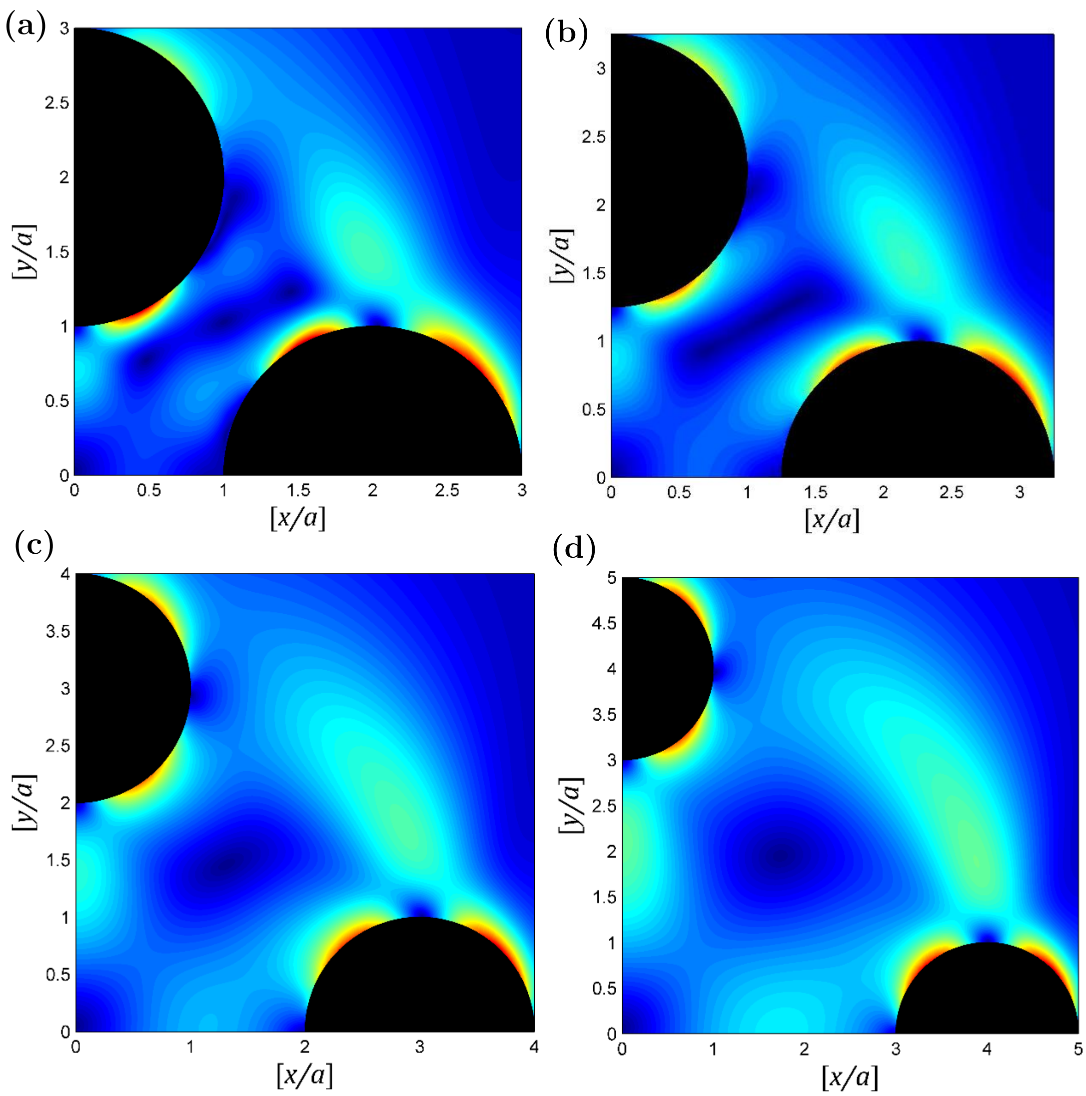

Figure 9. For ε=0.15, streaming velocity magnitude. (a)Cylinders located at a distance of two radius from reference frame (R2). (b) Cylinders located at a distance of two and a half radius from reference frame (R2.5). (c) Cylinders located at a distance of three radius from reference frame (R3). (d) Cylinders located at a distance of four radius from reference frame (R4)

Taking the R3 and R4 cylinder configurations, a simple test is done to choose the configuration to study it. Setting the previous parameters ($Re_s = 70$, $\varepsilon = 0.15$, $T \approx 0.2s$ and $a = 1cm$) and using as relative size of the inertial particle (b/a) the value of 0.175, the paths of the same particle placed in the same position (X-position=1cm and Y-position=1cm) with velocity equal to the surrounding fluid velocity, are sketched in *Figure 10* and *Figure 11* for both configurations.

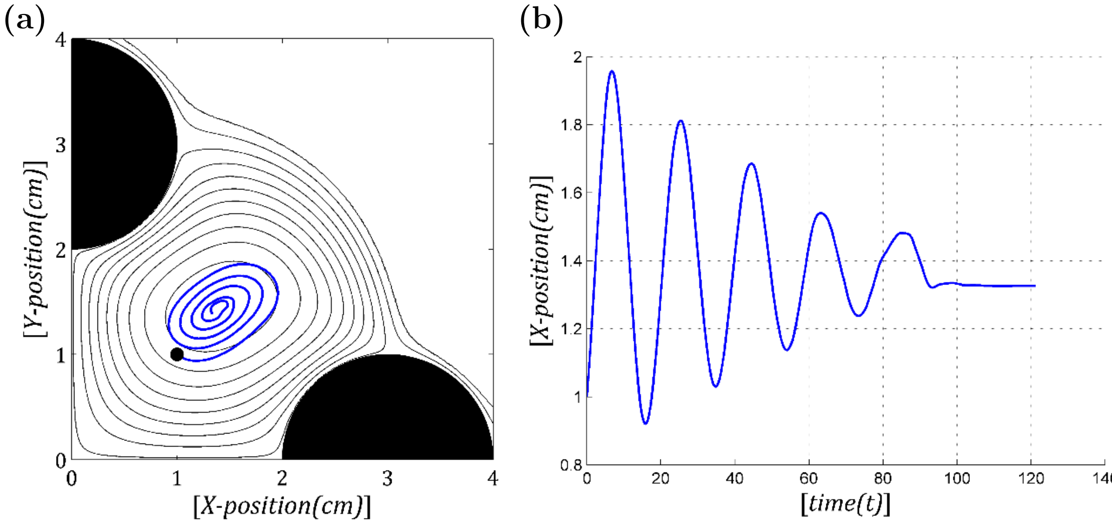

Figure 10. Inertial particle in the R3 cylinder configuration. (a) Trajectory when it is sampled once per period. (b) X-position when it is sampled once per period

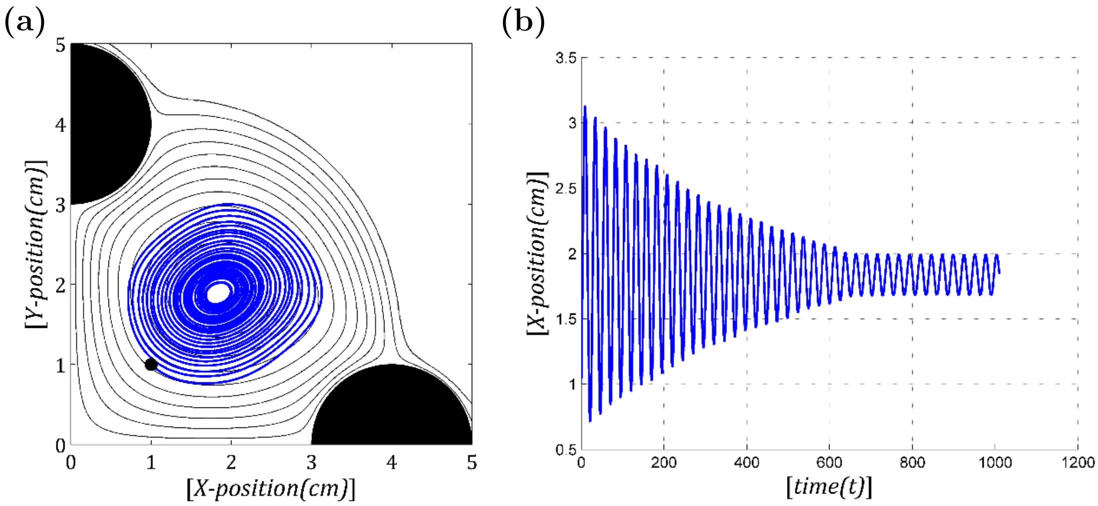

Figure 11. Inertial particle in the R4 cylinder configuration. (a) Trajectory when it is sampled once per period. (b) X-position when it is sampled once per period

In the R4 configuration, the inertial particle does not reach to be trapped, because the forces are not enough strong, and the particle will oscillate while in the

R3 configuration, the same particle is trapped in an effective way. Due to this reason, the chosen option is the R3 configuration.

3.4. Results

Keeping constant the R3 configuration with cylinder radius $a = 1cm$, this section provides the different effects of modifying the streaming Reynolds number, dimensionless oscillation amplitude, fluid to particle density ratio and the relative size of the inertial particle.

- **Changing streaming Reynolds number** (Re_s): the general tendency when this parameter increases, is to obtain greater trapping velocity, so in the same time the particle will reach the trapping position before.

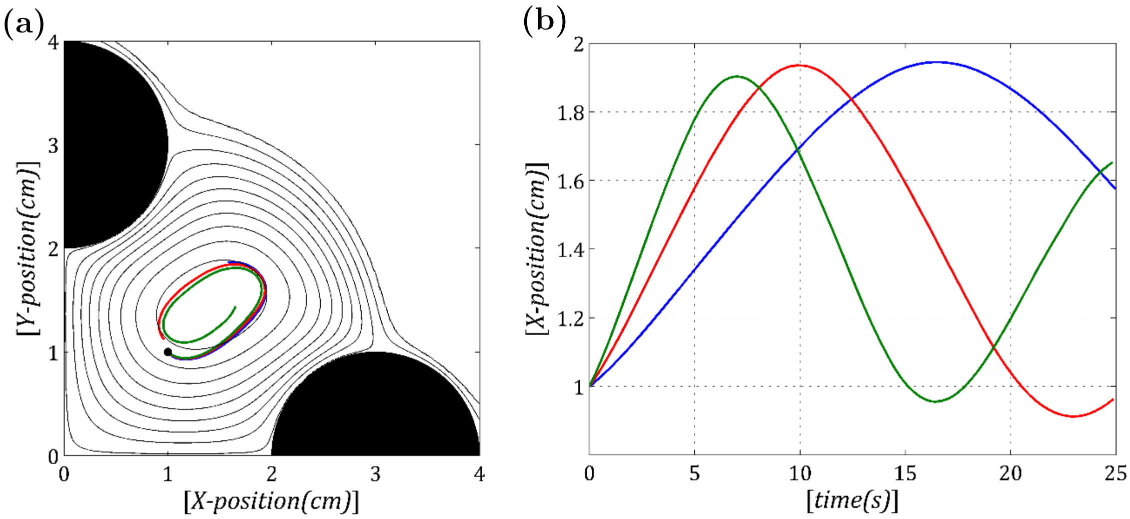

Figure 12. For ε=0.15, η=1 and b/a=0.175, changing the streaming Reynolds number: Res=30 (blue line), Res=50 (red line) and Res=70 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

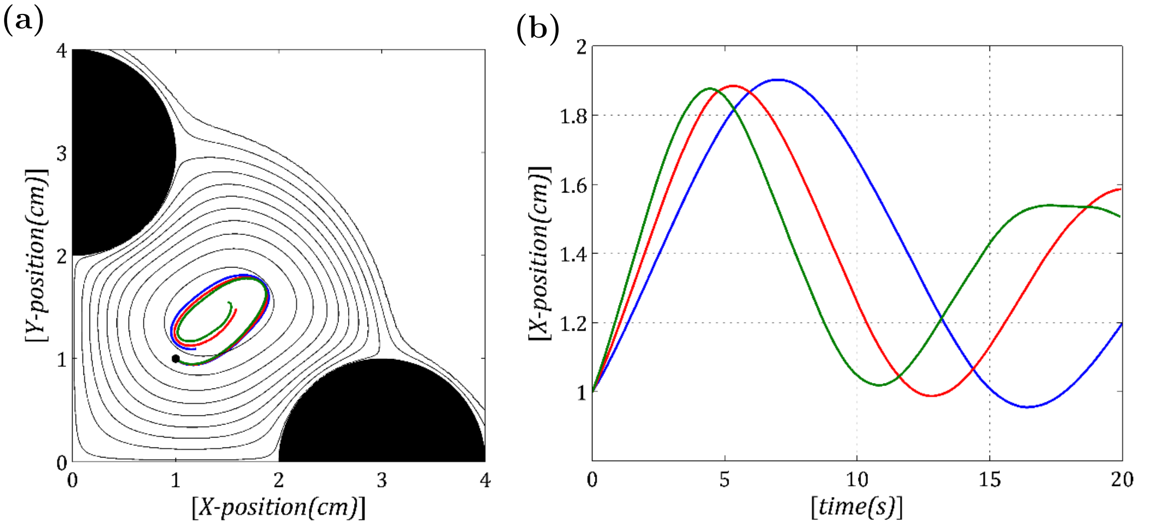

Figure 13. For ε=0.15, η=1 and b/a=0.175, changing the streaming Reynolds number: Res=70 (blue line), Res=90 (red line) and Res=110 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

- **Changing dimensionless oscillation amplitude** (ε): the normal tendency when this parameter increases, is inversely to the streaming Reynolds number effect, taking more time to trap the particle.

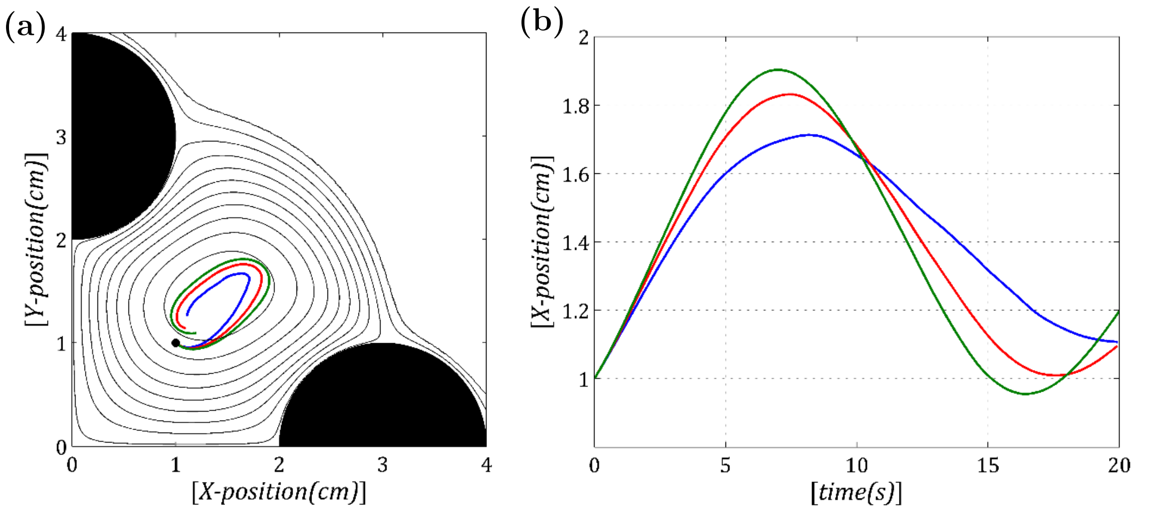

Figure 14. For Res=70, η=1 and b/a=0.175, changing the dimensionless oscillation amplitude: ε=0.1 (blue line), ε=0.125 (red line) and ε=0.15 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

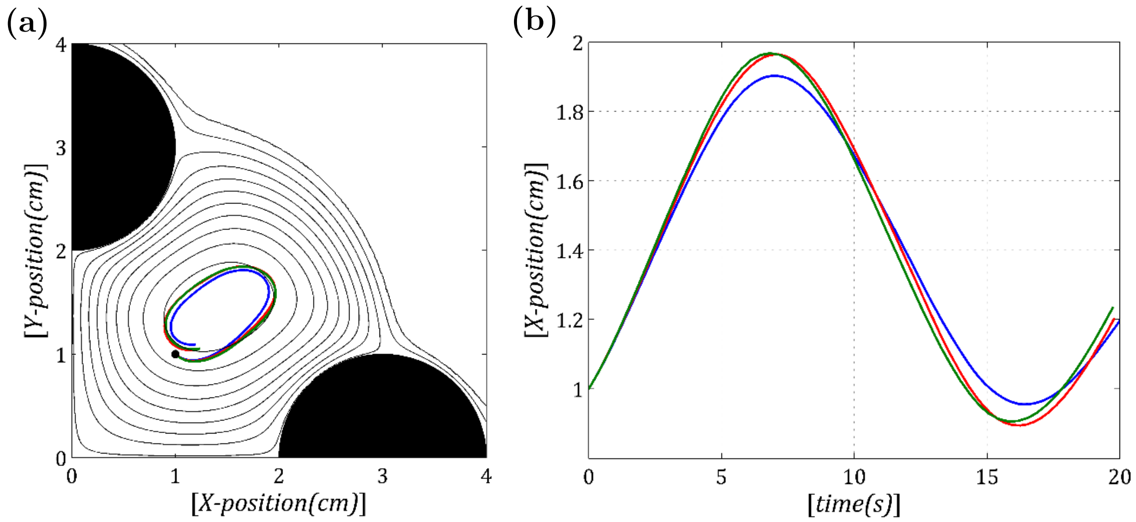

Figure 15. For Res=70, η=1 and b/a=0.175, changing the dimensionless oscillation amplitude: ε=0.15 (blue line), ε=0.175 (red line) and ε=0.2 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

- **Changing fluid to particle density ratio** (η): the general tendency when this parameter increases, is to change the path and decrease the amplitude around the trapping point.

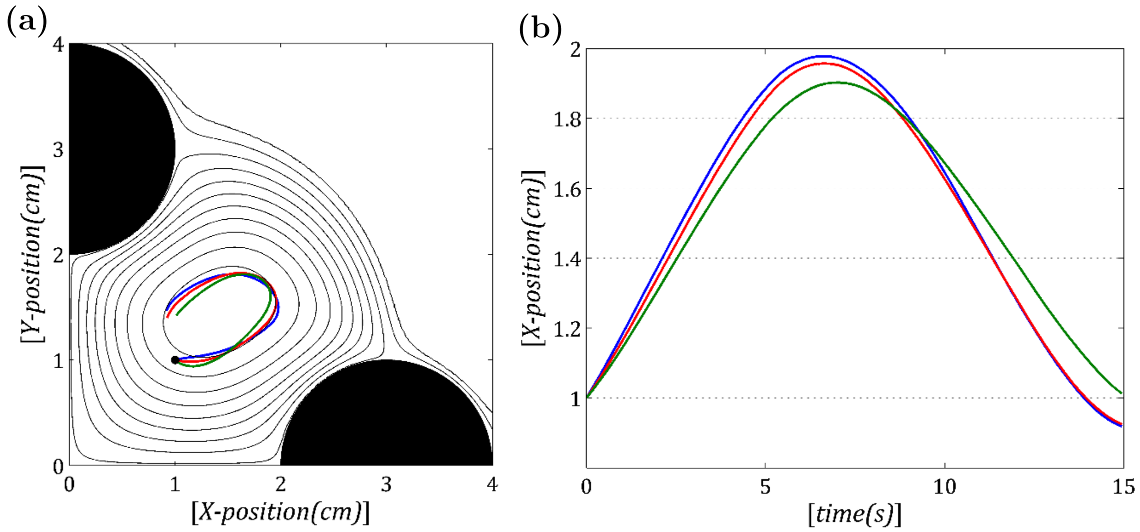

Figure 16. For Res=70, ε=0.15 and b/a=0.175, changing the fluid to particle density ratio: η=0.95 (blue line), η=0.975 (red line) and η=1 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

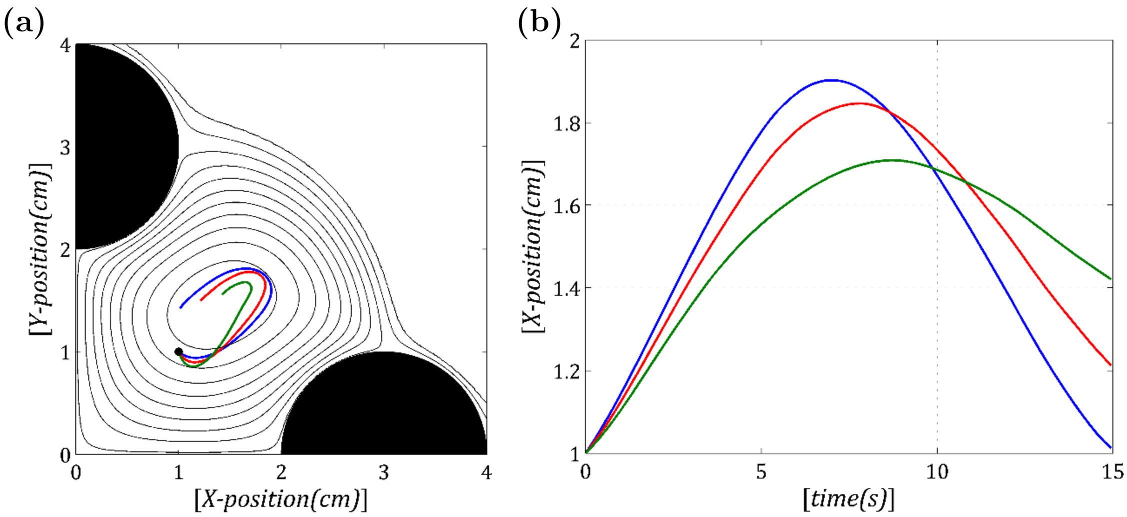

Figure 17. For Res=70, ε=0.15 and b/a=0.175, changing the fluid to particle density ratio: η=1 (blue line), η=1.025 (red line) and η=1.05 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

Now, the total time until inertial particle is trapped (time until the change in the position is almost negligible) is calculated. In addition the velocity magnitude, the Stokes number (equation 2.22) and the dimensionless thickness of the Stokes layer ($\delta/a = \varepsilon/\sqrt{Re_s} \ll 1$), are obtained.

η	Trapping time (s)	$U(m/s)$	St	δ/a
0.950	Not trapped	0.047	3.34	0.018
0.975	630	0.047	3.26	0.018
1.000	320	0.047	3.18	0.018
1.025	200	0.047	3.10	0.018
1.050	190	0.047	3.02	0.018

Table 3. For Res=70, ε=0.15 and b/a=0.175

- **Changing relative size of the inertial particle** (b/a): the general tendency when this parameter increases (the inertial particle is greater), is to reach the trapping position before.

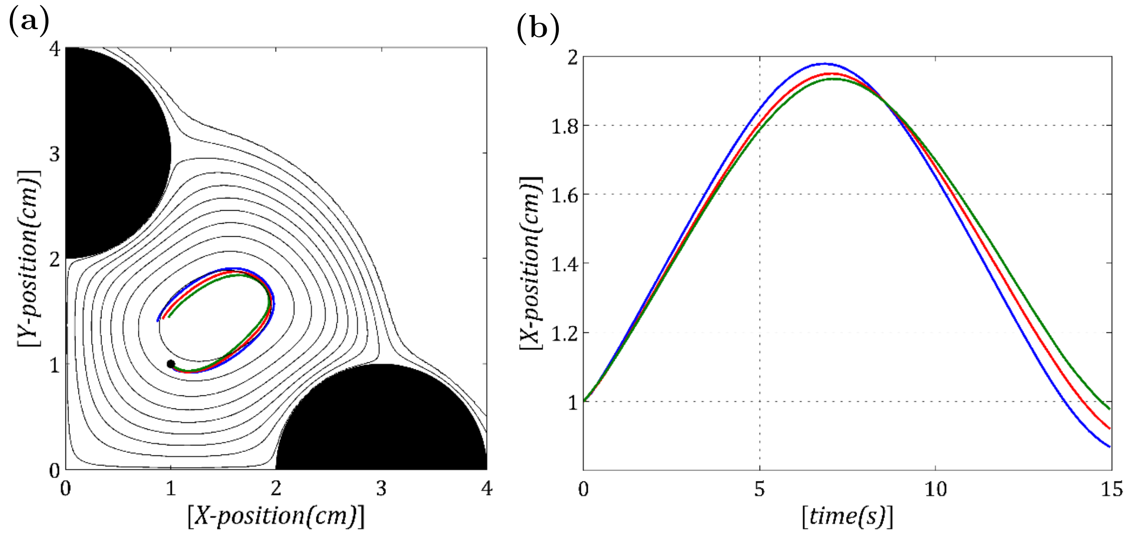

Figure 18. For Res=70, ε=0.15 and η=1, changing the relative size of the inertial particle: b/a=0.05 (blue line), b/a=0.1 (red line) and b/a=0.15 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

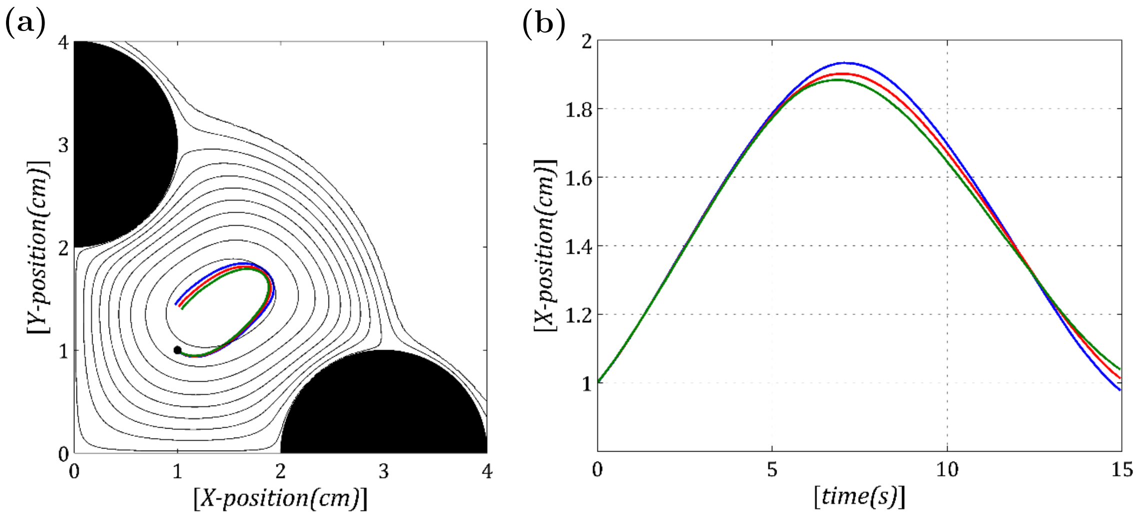

Figure 19. For Res=70, ε=0.15 and η=1, changing the relative size of the inertial particle: b/a=0.15 (blue line), b/a=0.175 (red line) and b/a=0.2 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period.

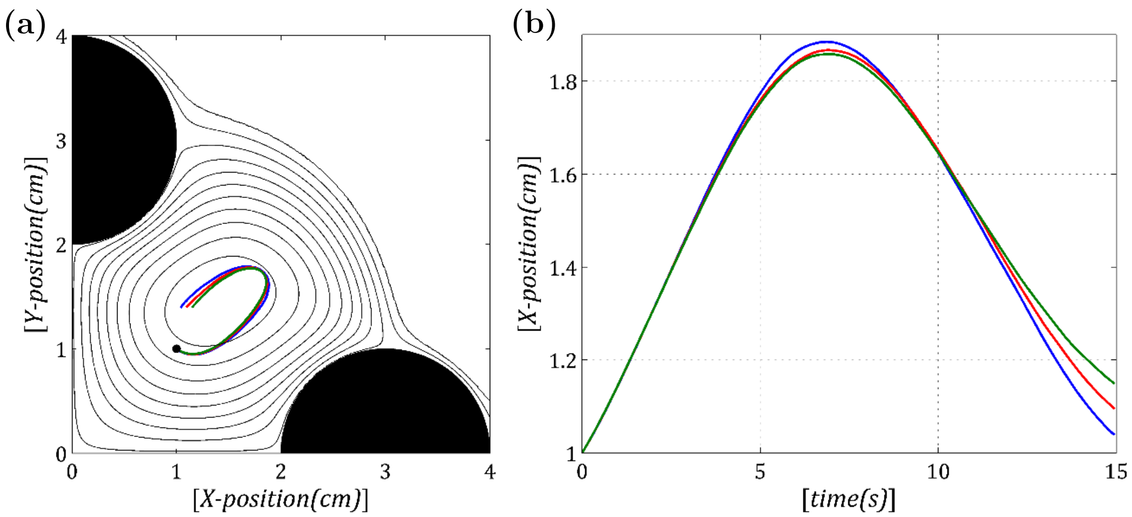

Figure 20. For Res=70, ε=0.15 and η=1, changing the relative size of the inertial particle: b/a=0.2 (blue line), b/a=0.225 (red line) and b/a=0.25 (green line). (a) Inertial particle trajectory when it is sampled once per period. (b) Inertial particle X-position deviation with time when it is sampled once per period

Now, the total times until inertial particle is trapped are calculated for different configurations in the parameters, keeping constant $\eta = 1$. The *not trapped* means that the inertial particle does not reach a fixed position and it only oscillates around the microeddy centre.

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	Not trapped	0.020	0.11	0.027
50	Not trapped	0.033	0.19	0.021
70	Not trapped	0.047	0.26	0.018
90	Not trapped	0.060	0.33	0.016
110	Not trapped	0.073	0.41	0.014

Table 4. For ε=0.15 and b/a=0.05

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	Not trapped	0.020	0.44	0.027
50	Not trapped	0.033	0.74	0.021
70	Not trapped	0.047	1.04	0.018
90	Not trapped	0.060	1.33	0.016
110	Not trapped	0.073	1.63	0.014

Table 5. For ε=0.15 and b/a=0.1

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	Not trapped	0.020	0.69	0.027
50	Not trapped	0.033	1.16	0.021
70	750	0.047	1.62	0.018
90	550	0.060	2.08	0.016
110	320	0.073	2.55	0.014

Table 6. For ε=0.15 and b/a=0.125

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	Not trapped	0.020	1.00	0.027
50	Not trapped	0.033	1.67	0.021
70	400	0.047	2.33	0.018
90	350	0.060	3.00	0.016
110	250	0.073	3.67	0.014

Table 7. For ε=0.15 and b/a=0.15

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	Not trapped	0.020	1.36	0.027
50	515	0.033	2.27	0.021
70	320	0.047	3.18	0.018
90	210	0.060	4.08	0.016
110	190	0.073	4.99	0.014

Table 8. For ε=0.15 and b/a=0.175

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	820	0.020	1.78	0.027
50	330	0.033	2.96	0.021
70	220	0.047	4.15	0.018
90	200	0.060	5.33	0.016
110	190	0.073	6.52	0.014

Table 9. For ε=0.15 and b/a=0.2

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	560	0.020	2.25	0.027
50	330	0.033	3.75	0.021
70	230	0.047	5.25	0.018
90	220	0.060	6.75	0.016
110	260	0.073	8.25	0.014

Table 10. For ε=0.15 and b/a=0.225

Re_s	Trapping time (s)	$U(m/s)$	St	δ/a
30	320	0.020	2.78	0.027
50	270	0.033	4.63	0.021
70	250	0.047	6.48	0.018
90	220	0.060	8.33	0.016
110	Not trapped	0.073	10.19	0.014

Table 11. For ε=0.15 and b/a=0.25

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	Not trapped	0.070	0.39	0.012
0.125	Not trapped	0.056	0.31	0.015
0.150	Not trapped	0.047	0.26	0.018
0.175	Not trapped	0.040	0.22	0.021
0.200	Not trapped	0.035	0.19	0.024

Table 12. For Res=70 and b/a=0.05

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	Not trapped	0.070	1.56	0.012
0.125	Not trapped	0.056	1.24	0.015
0.150	Not trapped	0.047	1.04	0.018
0.175	Not trapped	0.040	0.89	0.021
0.200	Not trapped	0.035	0.78	0.024

Table 13. For Res=70 and b/a=0.1

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	1100	0.070	2.43	0.012
0.125	Not trapped	0.056	1.94	0.015
0.150	750	0.047	1.62	0.018
0.175	Not trapped	0.040	1.39	0.021
0.200	Not trapped	0.035	1.22	0.024

Table 14. For Res=70 and b/a=0.125

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	660	0.070	3.50	0.012
0.125	530	0.056	2.80	0.015
0.150	420	0.047	2.33	0.018
0.175	Not trapped	0.040	2.00	0.021
0.200	Not trapped	0.035	1.75	0.024

Table 15. For Re=70 and b/a=0.15

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	460	0.070	4.76	0.012
0.125	340	0.056	3.81	0.015
0.150	320	0.047	3.18	0.018
0.175	400	0.040	2.72	0.021
0.200	300	0.035	2.38	0.024

Table 16. For Res=70 and b/a=0.175

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	340	0.070	6.22	0.012
0.125	330	0.056	4.98	0.015
0.150	200	0.047	4.15	0.018
0.175	Not trapped	0.040	3.56	0.021
0.200	210	0.035	3.11	0.024

Table 17. For Res=70 and b/a=0.2

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	460	0.070	7.88	0.012
0.125	340	0.056	6.30	0.015
0.150	220	0.047	5.25	0.018
0.175	210	0.040	4.50	0.021
0.200	190	0.035	3.94	0.024

Table 18. For Res=70 and b/a=0.225

ε	Trapping time (s)	$U(m/s)$	St	δ/a
0.100	620	0.070	9.72	0.012
0.125	260	0.056	7.78	0.015
0.150	240	0.047	6.48	0.018
0.175	220	0.040	5.56	0.021
0.200	190	0.035	4.86	0.024

Table 19. For Res=70 and b/a=0.25

CHAPTER 4

Conclusions and future works

4.1. Conclusions

In the project, many inertial particle trajectories have been calculated, varying the parameters that affect the equation of Maxey-Riley. Taking into account that the limitations for the FreeFem++ are that $\varepsilon \ll 1$ and the Stokes layer is small too ($\delta/a = \varepsilon/\sqrt{Re_S} \ll 1$), the main conclusion of the project are:

- The importance of the time step in the numerical method. Because of the fast oscillations of the flow, the time step should be enough small to represent all the oscillation variation, but the streaming velocity is of the order of εU so the total time to be trapped is large.
- Increasing the streaming Reynolds number (Re_S) produces greater trapping forces, so the total trapping time is decreased. The problem of high values of this parameter means that the flow is hard to control and any perturbation may produce turbulent issues. For slow values of Re_S, only relative big particles can be trapped while at high Re_S smaller inertial particles could be trapped too.

- About the fluid-to-particle density ratio η, as the value is greater, the trapping time is lower, so it is easier to capture particles with less density than the fluid.

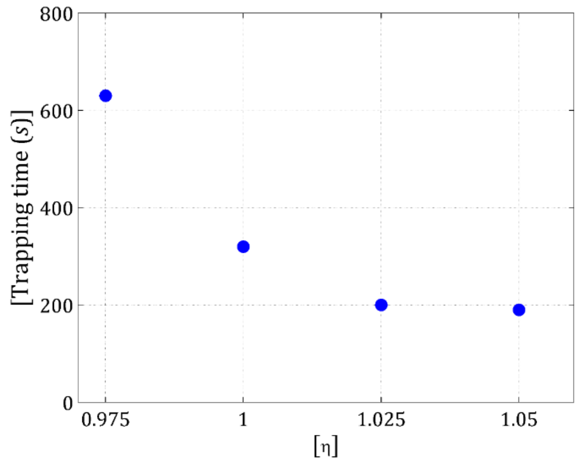

Figure 21. For Res=70, ε=0.15 and b/a=0.175

The limitations of this density parameter could be that if the particle is too heavy or too light, it will more difficult to keep the particle at the required level of the fluid and unwanted forces could be appear.

- Increasing the dimensionless oscillation amplitude (ε), the trapping force increases too, so the total time is decreased. This is a conclusion that contradicts the initial tendency described in the section 3.4.As this parameter is greater, only relative high inertial particles might be trapped. The limitations of this parameter are that the assumption made in the FreeFem++ and the consequence of being a big value could produce flow separation.
- Finally, seeing the variation of the Stokes number (St), which is a dimensionless parameter proportional to the inertia, the conclusion of that the particles with a Stokes number greater than 2 have high possibilities of being trapped.

4.2. Future works

This project could be continued in different ways: one of this, it would be to improve the numerical method, choosing smaller time step, and varying it not only depending on the period. It can be varied in a cosine way, taking more steps in the state of changing the directions of the oscillations, so accurate results would be obtained. Other work can be to do the experimental case with this cylinder configuration in order to validate the numerical method. This study can be done for different cylinder configurations and parameters, so the conclusions obtained could be used for build a machine which could filter the particles depending of their size.

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